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NUMERICAL INVESTIGATION OF DEFORMATIONS OF PLANAR FLEXOELECTRIC NEMATIC LAYERS CONTAINING IONS

Deformations of planar nematic layers of conducting nematic liquid crystal possessing flexoelectric properties and subjected to external d.c. voltage were studied numerically. Various kinds of electrodes, from strongly blocking to well conducting, were assumed. The calculations were performed for nematic material characterized by positive dielectric anisotropy and by positive sum of flexoelectric coefficients. The threshold voltages for deformations were computed for various ion concentrations and for several rates of electrode processes. The enhancement as well as reduction of the threshold were observed. Well defined dependence of layer behaviour on the kind of electrodes and on the ion concentration was found. These effects are due to interactions between flexoelectric polarization and strong electric field of high gradient.

Keywords: nematics, flexoelectricity.

1. INTRODUCTION

The d.c. electric field applied to liquid-crystalline layer induces elastic deformations, which are manifested by changes of director distributions. These deformations are consequence of dielectric anisotropy and of flexoelectric properties of a nematic material. Their character depends also on ion contents in the nematic. The origin of flexoelectric properties is bending of molecules and different structure of their ends. The external electric field interacts with dipole moments of molecules which induces deformation.

The deformation induced by electric field applied perpendicular to the layer has threshold character. The value of threshold voltage depends on dielectric and flexoelectric properties as well as on ion contents and on kind of electrode contacts. These parameters influence the electric field distribution and in consequence the form of deformations.

Our aim was to study numerically the influence of ion contents and kind of electrode contacts on deformations of planar layer containing a conducting nematic characterized by positive dielectric anisotropy and positive sum of flexoelectric coefficients. As a result, the threshold voltage, the director configurations and the electric field distributions were determined.

2. GEOMETRY, PARAMETERS AND METHOD

An infinite planar nematic layer of thickness $d = 20$ μm confined between two electrodes parallel to the xy-plane, positioned at $z = -d/2$ and $z = d/2$, was considered. The surface anchoring was of moderate strength $W = 2\cdot 10^{-5}$ J/m^2 and it was identical on both boundaries. The typical values of the elastic constants were assumed, $k_{11} = 4.3$ and $k_{33} = 8.6$ pN. The flexoelectric properties were determined by the sum of flexoelectric coefficients $e_{11}+e_{33} = 40$ pC/m and the dielectric properties by dielectric constants $\varepsilon_{\parallel} = 7.4$ and $\varepsilon_{\perp} = 5.4$. The transport of ions within the layer was described by their mobilities and by the diffusion coefficients. It was assumed that the mobility of positive ions was ten times lower than that of the negative ions. The corresponding components of the mobility tensor were $\mu_{\parallel}^{-} = 1.5\cdot 10^{-9}$, $\mu_{\perp}^{-} = 1\cdot 10^{-9}$, $\mu_{\parallel}^{+} = 1.5\cdot 10^{-10}$ and $\mu_{\perp}^{+} = 1\cdot 10^{-10}$ m^{2}V^{-1}s^{-1}. The diffusion coefficients were determined by the Einstein relation $D_{\parallel,\perp}^{\pm} = (k_B T/q)\mu_{\parallel,\perp}^{\pm}$, where k_B is the Boltzmann constant, T is the absolute temperature and q denotes the absolute value of the ionic charge. The electrical properties of the nematic were described by means of dissociation constant β and recombination constant α in accordance with the weak electrolyte model [1]. The recombination constant was calculated from the Langevin formula [2]: $\alpha = 2q\bar{\mu}/\varepsilon_0\bar{\varepsilon}$, where the average quantities were expressed by $\bar{\mu} = \left[\left(2\mu_{\perp}^{+} + \mu_{\parallel}^{+}\right)/3 + \left(2\mu_{\perp}^{-} + \mu_{\parallel}^{-}\right)/3\right]/2$ and $\bar{\varepsilon} = \left(2\varepsilon_{\perp} + \varepsilon_{\parallel}\right)/3$. The dissociation constant β depended on the electric field strength E according to the Onsager theory [2]: $\beta = \beta_0\left(1 + q^3 E/8\pi\varepsilon_0\bar{\varepsilon}k_B{}^2T^2\right)$. Suitable values of β_0 were chosen in order to obtain the required average ion concentrations.

In this paper, we report the results obtained for several kinds of electrode contacts for which the transport of ions across the nematic-electrode contact was significantly limited by energy barriers which determined the kinetics of corresponding electrochemical reactions. For this purpose we have used a simplified model proposed in earlier papers [3,4,5].

In this approach, the electrode contacts were characterized by the coefficients k_r which expressed the rates of generation and neutralization of ions. Their values ranged from 10^{-7} to 10^{-3} m/s for strongly blocking and well conducting contacts respectively.

The state of flexoelectric nematic layer subjected to the external electric field is described by the set of ten equations which consists of a torque equation for the bulk, two torque equations for the boundaries, an electrostatic equation, two equations of continuity of anions and cations fluxes in the bulk and four equations describing the boundary conditions for ion transfer across the electrode contacts [3]. The numerical solution of these equations yields the functions $\theta(z)$, $V(z)$ and $N^{\pm}(z)$ which determine the director configuration, the electric potential distributions and the ion concentrations respectively, for various voltages and generation constants β_0. These results allowed us to determine the threshold voltages U_T for the deformations which are presented in the following.

3. RESULTS

In the following, the results concerning the threshold voltage, the director configurations and the electric field distributions will be divided into three parts corresponding to three ranges of average ion concentrations, N_{av}, namely low, moderate and high.

3.1. Threshold voltage

The threshold voltage values obtained for various ion concentrations and several rates of electrode processes are presented in Fig. 1. It is evident that the value of threshold voltage for strongly blocking or weakly conducting electrode contacts, $k_r = 10^{-7}$ - 10^{-5} m/s, reaches a maximum of ca. 4 V in the range of intermediate concentrations, N_{av}~10^{19} m^{-3}.

In the case of conducting contacts, $k_r = 10^{-3}$ m/s, the value of threshold voltage is close to the theoretical value, [6], U_f =1.8 V and does not depend on ion concentration.

For low ion concentrations, $N_{av} < 10^{18}$ m^{-3}, the threshold voltage ranges from 1.8 to 3 V. Higher values from this range appear for the well and weakly conducting electrodes.

In the range of intermediate ions concentrations, the threshold voltage for weakly conducting electrode contacts increases rapidly. For the layer with strongly blocking electrodes, $k_r = 10^{-7}$ m/s, its maximum is shifted towards the higher ion concentrations.

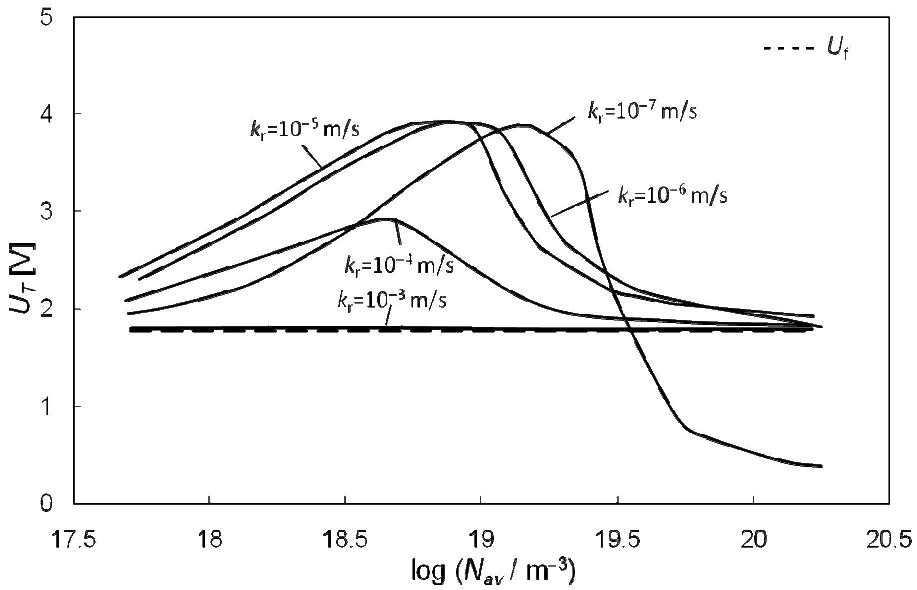

Fig. 1. Threshold voltage U_T as a function of average ion concentration N_{av}, for severalvalues of k_r indicated at curves . The dotted line denotes U_f value

For high ion concentrations, the threshold voltage approaches the theoretical value $U_f = 1.8$ V if $k_r \geq 10^{-6}$ m/s. For strongly blocking electrode contacts, $k_r = 10^{-7}$ m/s, the threshold rapidly decreases to very low value of ca. 0.3 V.

3.2. Director distributions

Figures 2-4 present the director distributions for low, moderate and high ion contents respectively. They were calculated for the voltage exceeding the threshold by 0.1 V: $U = U_T + 0.1$ V.

At low ion contents, the deformation is symmetrical (Fig. 2). The largest director deviation occurs in the middle of layer, whereas at the walls the deformation decreases. The director distribution is close to that which occurs in a layer of non-conducting nematic devoid of flexoelectric properties. The role of flexoelectric properties manifests itself only by slight asymmetry of deformation.

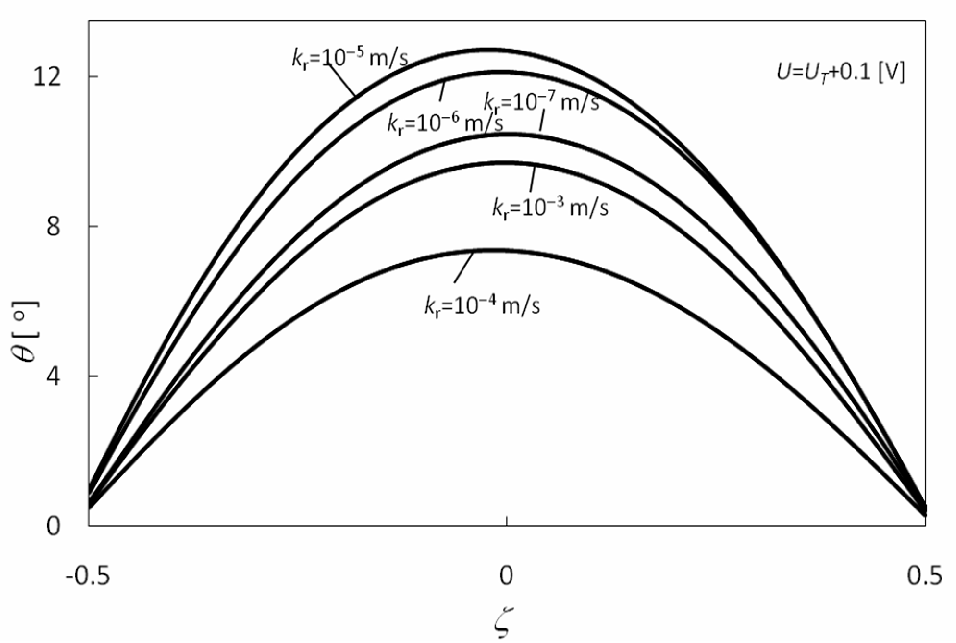

Fig. 2. Director profiles θ as a function of the reduced coordinate ζ for low ion concentrations. k_r in ms^{-1} are indicated at curves

In the range of intermediate ions concentrations (Fig. 3), the dependence of deformation character on the conductivity of contacts is revealed. For the well conducting contacts, the deformation has still symmetrical shape, whereas deviation from this symmetry is observed for the blocking electrodes. The deformations are much higher at the electrode of lower potential and slightly decrease in the neighbourhood of this contact. In the case of well conducting contact, the distribution is still symmetric.

For high ion concentrations and strongly blocking contacts, $k_r = 10^{-7}$ m/s, (Fig. 4), the director distribution is asymmetrical: the angle describing director deviation is small at cathode, increases linearly along the layer normal and decreases in the close vicinity of anode. In the case of well and weakly conducting electrodes, the director distribution is nearly symmetrical.

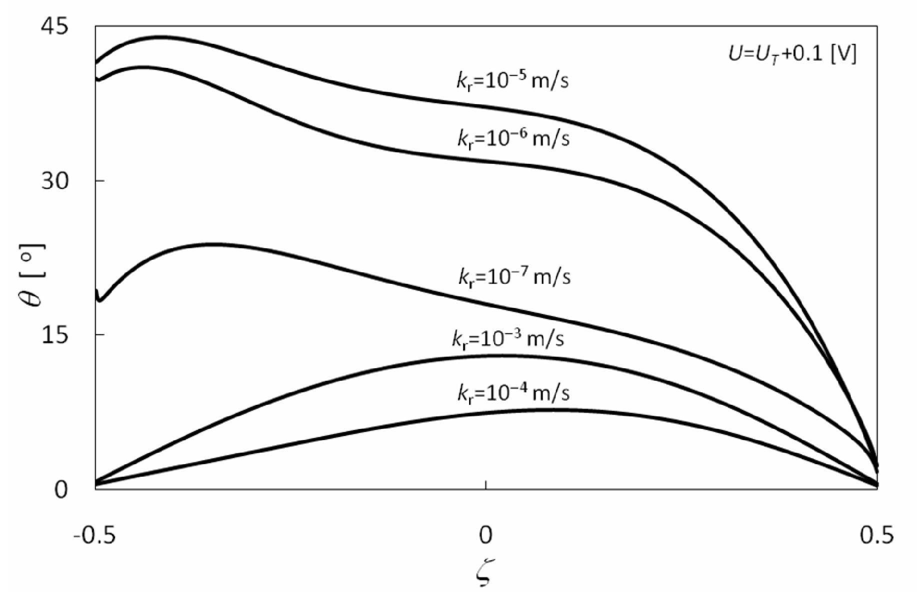

Fig. 3. Director profiles θ as a function of the reduced coordinate ζ for intermediate ion concentrations. k_r in ms^{-1} are indicated at each curve

3.3. Electric field distributions

The electrical field inside the layer (figures 5-7) is determined by ionic space charge distribution. At all investigated ion concentrations, the electric field in the layer with conducting contacts is practically constant over the whole thickness. Lower rate of electrode processes causes accumulation of ions at the electrodes. In consequence, the distribution of electric field varies strongly in these areas. Higher transmission of electrode contacts creates smaller gradient of electric field.

In the case of low ion concentrations (Fig. 5), for intermediate speed of ions neutralization ($k_r = 10^{-6} - 10^{-4}$ m/s), electric field increases at negative electrode and the field gradient is relatively small. At strongly blocking electrodes, $k_r = 10^{-7}$ m/s, increase of electric field is visible in thin sub-electrode layers.

For intermediate ion concentrations (Fig. 6), and for weakly conducting or strongly blocking contacts, asymmetry of director distribution reveals. The electric field gradient is limited to the negative half of the layer.

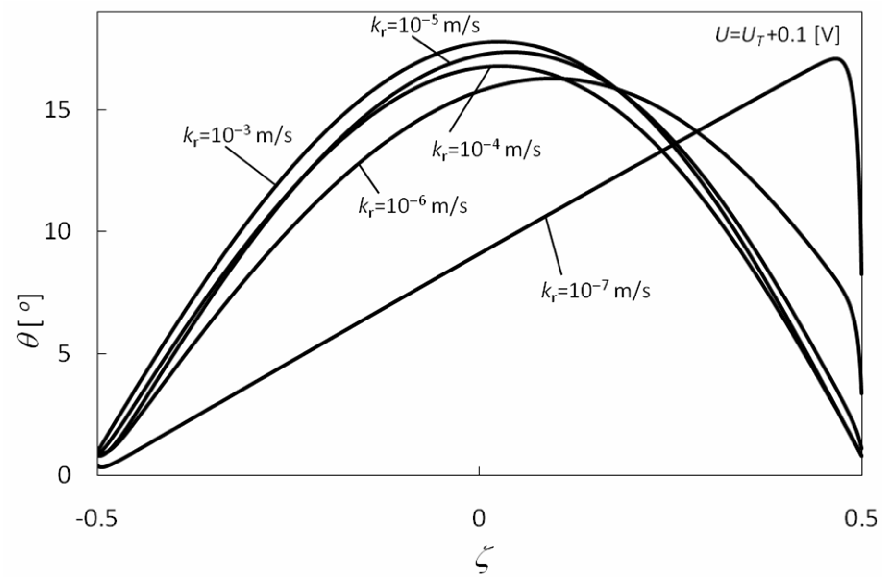

Fig. 4. Director profiles θ as a function of the reduced coordinate ζ for high ion concentrations. k_r in ms^{-1} are indicated at each curve

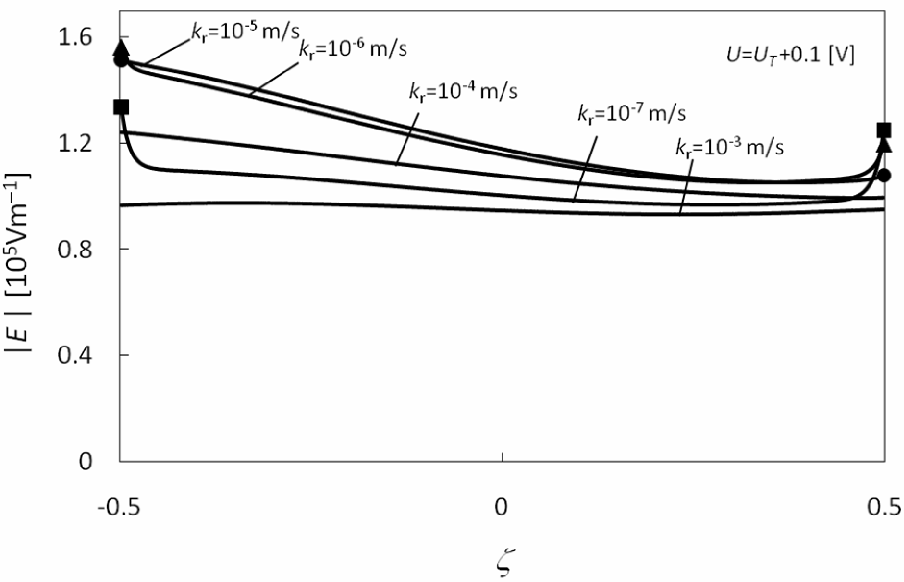

Fig. 5. Electric field strength $|E|$ as a function of the reduced coordinate ζ for low ion concentrations. k_r in ms^{-1} are indicated at at each curve

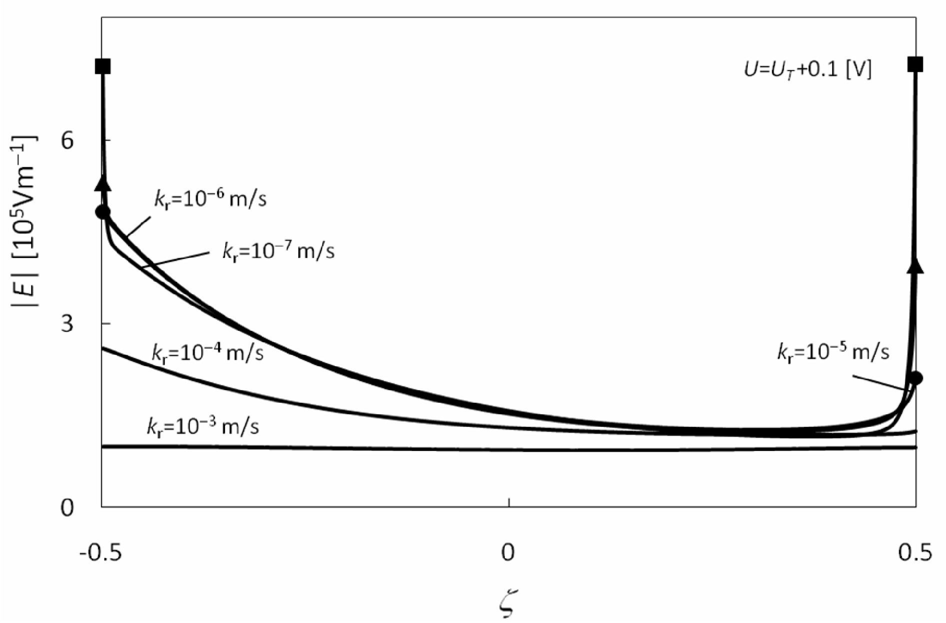

Fig. 6. Electric field strength |*E*| as a function of the reduced coordinate ζ for intermediate ion concentrations. k_r in ms^{-1} are indicated at curves

For high ion concentrations (fig. 7), electric fields and electric field gradients are very strong already at $k_r = 10^{-6}$ m/s. Strongly blocking electrodes ($k_r \le 10^{-6}$ m/s) cause that electric field at boundaries of the layer reaches significant values. In thin subelectrode regions (of thickness c.a. 0.03*d*), the electric field is hundred times higher than in the bulk. This effect is the more pronounced, the stronger is blocking character of the electrode contacts. For well conducting electrodes, the electric field is constant over the whole layer thickness.

5. DISCUSSION

Deformations of nematic layer are determined by dielectric and flexoelectric properties. They depend on kind of electrode contacts and on ion concentrations. Flexoelectric properties exert essential influence on behaviour of the layer in electric field only when the electrode contacts have blocking character. This is connected with high electric field and electric field gradient in the vicinity of electrodes. On the other hand, fast electrode process result in

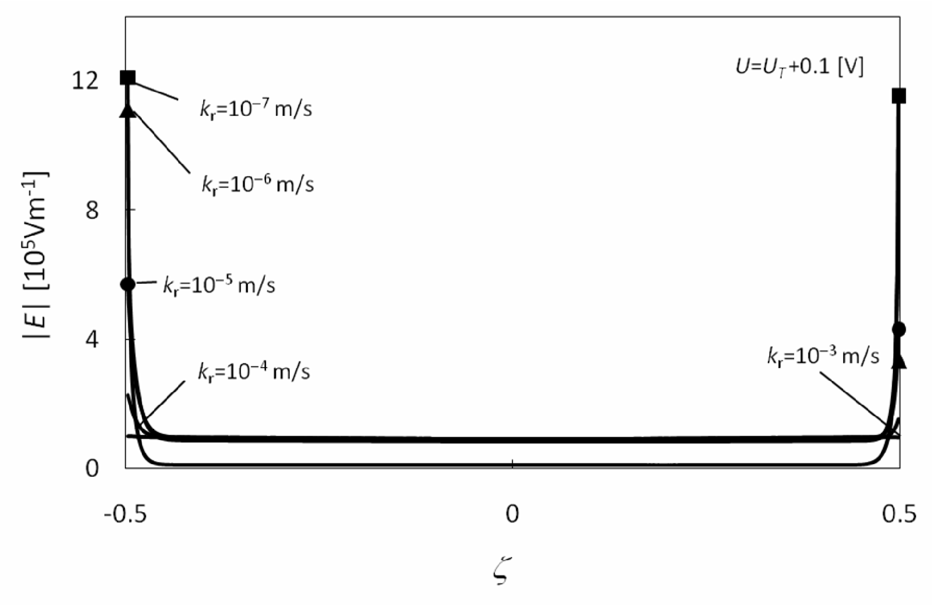

Fig. 7. Electric field strength |*E*| as a function of the reduced coordinate ζ for high ion concentrations. k_r in ms^{-1} are indicated at each curve

equalization of ion concentration in all the bulk of the layer and the electric field is therefore uniform.

Deformations taken into account in this paper are one-dimensional. This means, the all physical quantities describing them depend only on one coordinate z measured along the normal to the layer plane. However, in the planar flexoelectric nematic layers subjected to the electric field applied perpendicular to the layer, two-dimensional deformations are possible. The physical quantities which describe them vary along two directions: along the z axis and along the coordinate parallel to the layer plane and perpendicular to the easy axis. The dependence of the angle θ on this coordinate is periodical which causes that periodic patterns are seen in the layer under a microscope between crossed polarizers. They are known as longitudinal domains or Vistin domains. They are parallel to the initial orientation of director. Their width is comparable with the thickness of the layer. This kind of spatially periodical deformations is possible if the flexoelectric effects prevail over the dielectric effects. This criterion is expressed by inequality

$$(e_{11} - e_{33})^2 > \varepsilon_0 |\Delta\varepsilon| k \qquad (1)$$

which is obtained under assumption that $k_{11} = k_{22} = k_{33} = k$ [7]. In the present paper, both flexoelectric coefficients are equal $e_{11} = e_{33}$ = 20 pC/m. This means that $e_{11} - e_{33} = 0$, and periodical deformations are absent.

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NUMERYCZNE BADANIE ODKSZTAŁCEŃ PLANARNYCH WARSTW FLEKSOELEKTRYCZNYCH NEMATYKÓW ZAWIERAJĄCYCH JONY

Streszczenie

Przedstawiono wyniki symulacji numerycznych dotyczących zachowania planarnej warstwy przewodzącego nematyka posiadającego właściwości fleksoelektryczne i poddanego działaniu zewnętrznego stałego napięcia. Badana warstwa była scharakteryzowana poprzez dodatnią sumę współczynników fleksoelektrycznych oraz dodatnią wartość anizotropii dielektrycznej. Uwzględniono przepływ prądu przez warstwę w przypadkach elektrod słabo i silnie blokujących oraz dobrze i słabo przewodzących. Napięcia progowe na powstanie deformacji są zaprezentowane dla kilku szybkości procesów przyelektrodowych. Obserwowano zarówno podwyższenie jak i obniżenie wartości progu. Określono zależność zachowania warstwy od rodzaju elektrod i koncentracji jonów. Za przyczynę zaobserwowanych zjawisk można uznać oddziaływanie polaryzacji fleksoelektrycznej z polem elektrycznym o dużym natężeniu i gradiencie.